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MgO/Fe(100) Interface: A Study of the Electronic Structure

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Single crystalline magnetic tunnel junctions based on the Fe/MgO interface have shown significant advantages over earlier structures using Al_2O_3 barrier. However, according to recent theoretical results, their performance might be compromised by the interfacial FeO layer, the existence of which has been reported in experimental x-ray diffraction studies. We have prepared epitaxial MgO/Fe(001) interfaces and performed in-situ spin-polarized angle-resolved photoemission studies on them. The electronic signature of the FeO layer at the interface has not been found, thus existence of such a layer is not an intrinsic property of MgO/Fe interfaces.

In recent years, there have been significant advances in the preparation of single crystalline magnetic tunnel junctions (MTJs) based on MgO(100)-insulating barriers. For example, the theoretically predicted tunneling magnetoresistance (TMR) of several hundred percent in Fe/MgO/Fe(100) has been experimentally verified with values of 180 - 220% for room temperature and even higher values are being reported for various other electrode compositions. However, several theoretical studies have predicted that the oxidation of the MgO/Fe contacts is detrimental to the performance of these MTJs.

Figure 1 shows how annealing of the MgO/Fe(001) interface influences the valence band spectra. In these spectra, Fe 3d-related features appear between 0-4 eV binding energy, while MgO-related features appear for binding energies above 4 eV. Annealing up to 400°C begins to sharpen Fe 3d spectral features in the region close to the Fermi edge and this process is even more visible in the 500°C spectrum, where the sharp spectral feature of the clean Fe surface is nearly fully recovered (right panel in **Figure 1**). This is a clear indication of the absence of the FeO interlayer.

Further poof is obtained by studying core level spectra. The Fe 3p levels exhibit a large magnetic linear dichroism (MLD) in photoemission that can be used to monitor the magnetic state of the Fe layer. Binding energies of Fe 3p and Mg 2p are similar and dichroic spectra in this region are present in **Figure 2**. Comparing spectra from the clean Fe(100) surface (**Figure 2(a)**) to the ones exposed intentionally to 1 Langmuir (L) of molecular oxygen (**Figure 2(b)**), the appearance of a shoulder on the high binding energy side of the spectrum is evident. This shoulder feature, best seen in the right panel of **Figure 2**, is typical of a reaction of oxygen with Fe and indicates the formation of Fe oxide. This shoulder does not display any dichroism, indicating the formation of an unpolarized surface oxide upon even 1 L of oxygen exposure to the clean Fe surface. Most importantly, when MgO is deposited on clean Fe(001) instead (**Figure 2(c)**), there is no indication of this feature in the spectra. On the contrary, the curvature of the relevant part of the core level spectrum remains clearly positive for 1 ML MgO coverage, which is further evidence that no FeO layer is present at the MgO(100)/Fe(100) interface. At higher MgO deposition, the Fe 3p emission becomes rapidly obscured by the much more intense Mg 2p levels (**Figures 2(c)-(d)**) but the Fe dichroism remains strong, which indicates a highly polarized Fe substrate in contact with the MgO overlayer. It is also useful to note that while the Fe dichroism is very strong, no sign of any dichroism is detected under the Mg peak (the full dichroic spectra are shown in the left panel for the case 0.5 ML MgO, as an example). This again

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tends to confirm the low interaction between Fe and MgO at the interface. For thicker films, where no Fe signal remains, there is no additional Mg 2p line related to metallic Mg. Such a metallic feature would be expected to appear at 2 eV lower binding energy than the main 2p line of MgO, and its complete absence is a confirmation of the good stoichiometry of these films.

In conclusion, by measuring angle- and spin-resolved photoemission spectra we have observed no signs of FeO in our films. Thus, electronically, our samples represent a sharp interface between Fe and MgO, where Fe does not get oxidized during the MgO deposition, i.e. we did not find electronic signature of interfacial FeO layer.

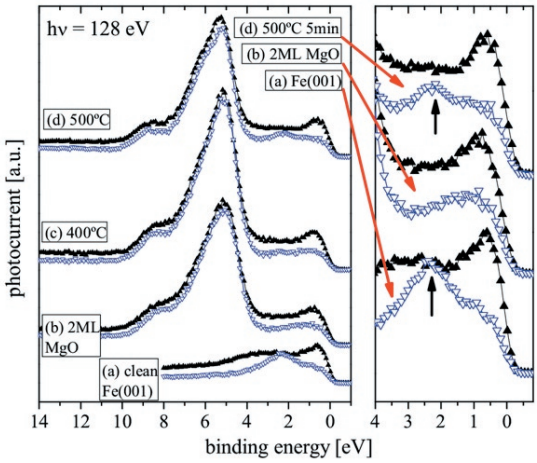

Figure 1. *Spin-polarized photoemission spectra at hν = 128 eV. Left panel: (a) clean Fe(100) (b) 2 ML of MgO/Fe(100) (c) annealed to 400°C for 5 min (d) subsequently annealed to 500°C for 5 min. In right panel, selected spectra are magnified in the region close to the Fermi edge. Spectra are normalized to the majority spin Fe-related part near the Fermi edge. All spectra were taken at room temperature.*

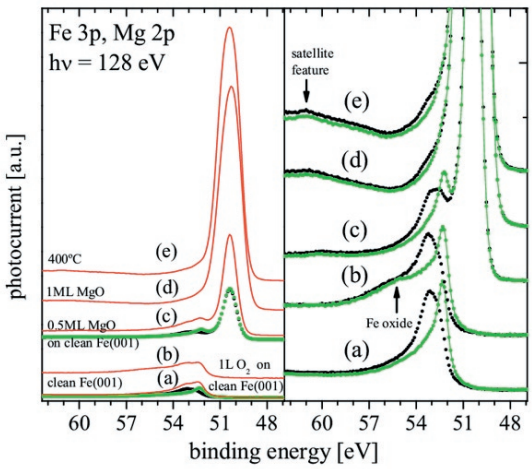

Figure 2. *Fe 3p and Mg 2p core level spin-integrated normal emission energy distribution curves at hν = 128 eV; (a) clean Fe(001), (b) Fe(001)exposed to 1L of molecular oxygen, (c) 0.5ML MgO/Fe(001) deposited on clean Fe(001), (d) 1ML MgO/Fe(001), (e) previous films annealed to 400°C for 5 min. In the left panel, the sum of spectra from the sample magnetized in opposite directions are plotted. The right panel shows the same spectra as on the left but renormalized to magnify the Fe 3p contribution. Opened and closed circles represent spectra from the sample magnetized in opposite directions. All spectra were measured at room temperature.*